

1,2,3,5-Tetrachlorobenzene
634-90-2 | DTXSID1026089

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 235 °C

Global applicability domain: Inside

Local applicability domain index: 6.86e-01

Confidence level: 9.14e-01

Nearest Neighbors from the Training Set

Image not found

Benzene, 1-bromo-3,5-dichloro-

Measured: 232

Predicted: 229

Image not found

Benzene, 4-bromo-1,2-dichloro-

Measured: 237

Predicted: 229

Image not found

Benzene, 2-bromo-1,4-dichloro-

Measured: 226

Predicted: 229

Image not found

2,5-Dibromotoluene

Measured: 236

Predicted: 233

Image not found

1-Bromo-2,3-dichlorobenzene

Measured: 245

Predicted: 229